Name: _____

PHYSICS 619 : SPRING SEMESTER 2019

HW #12: Diffusion Monte Carlo (DMC) with importance sampling

1.) Compute the exact ground state energy of the Helium atom by use of the Diffusion Monte Carlo algorithm with importance sampling. Use the trial function introduced in problem 3 of HW7. Read Moskowitz et al, J. Chem. Phys. 77(1982)349, S. A. Chin, Phys. Rev. 42(1990)6991. Not all the materials in these two paper are equally relevant.

The basic idea of DMC is to use the Langevin algorithm to iterate the configurations of the system (the two electrons' position in the case of Helium), but ADDITIONALLY, replicated each configuration according to the exponential of the local energy as described in the lecture note. When computing the energy expectation values, average over ALL configurations (include those replicated ones).

This is the last assignment of the course and will due on the last day of class.